

# Diabatic and Adiabatic Collective Motion in a Model Pairing System

Takashi Nakatsukasa\* and Niels R. Walet†

*Department of Physics, UMIST, P.O.Box 88, Manchester M60 1QD, UK*

## Abstract

Large amplitude collective motion is investigated for a model pairing Hamiltonian containing an avoided level crossing. A classical theory of collective motion for the adiabatic limit is applied utilising either a time-dependent mean-field theory or a direct parametrisation of the time-dependent Schrödinger equation. A modified local harmonic equation is formulated to take account of the Nambu-Goldstone mode. It turns out that in some cases the system selects a diabatic path. Requantizing the collective Hamiltonian, a reasonable agreement with an exact calculation for the low-lying levels are obtained for both weak and strong pairing force. This improves on results of the conventional Born-Oppenheimer approximation.

PACS number(s): 21.60.-n, 21.60.Ev

Typeset using REVTeX

---

\*Electronic address: T.Nakatsukasa@umist.ac.uk

†Electronic address: Niels.Walet@umist.ac.uk

## I. INTRODUCTION

Nuclei are finite fermionic many-body systems which support many kinds of collective motion. While properties of high-frequency vibrations (giant resonances) may be well reproduced in the small-amplitude limit by the random-phase approximation (RPA), some low-frequency vibrations exhibit a strongly anharmonic nature that the RPA cannot describe. Nuclear fission and shape coexistence phenomena also have such a large amplitude nature. In order to investigate these kinds of large amplitude collective motion, one would like to reduce the number of degrees of freedom to a few judiciously chosen slow collective coordinates. However, in nuclear systems, this task is not trivial, since there is no obvious separation of scales.

In molecular physics, where the masses of electrons are so much smaller than those of the atomic nuclei, the electronic motion is normally much faster than nuclear motion. Thus, the collective coordinates are usually functions of nuclear coordinates and the Born-Oppenheimer (BO) approximation works very well. On the other hand, in nuclear physics, since a nucleus consists of neutrons and protons which have almost the same masses, both the definition of collective coordinates and the applicability of adiabatic assumption are never obvious.

Although a large number of studies have been done to calculate the potential energy surface using the constrained Hartree-Fock (HF) or Hartree-Fock-Bogoliubov (HFB) theory with a given generalised cranking (or constraint) operator, the choice of collective coordinate (i.e., the choice of cranking operators) has been rather arbitrary in most cases.

In this paper we shall apply a special theory [1], that is designed to determine a self-consistent cranking operator for adiabatic large amplitude collective motion (ALACM). This theory provides a method to find approximate decoupled motion which is confined to a few dimensional submanifold of the configuration space, within the framework of classical Hamiltonian dynamics. Since most systems of practical interest are not exactly separable, it is important that the theory can provide a submanifold which is approximately decoupled. This method has been applied to problems in nuclear physics [2,3] and in other fields (see references in [1])

In nuclear collective motion which involves level crossings, the problem of adiabaticity versus diabaticity has been a long standing question since this problem was discussed by Hill and Wheeler [4]. During a nuclear shape change, the diabatic process is often more favoured than the adiabatic one [5]. This raises the question whether an *adiabatic* theory, such as ALACM, can be used to shed some light on diabatic dynamics. An answer to this question is one of main goals of this paper.

In nuclear phenomena, it is well-known that the pairing (superfluidity) influences all low-frequency collective motion. A well-known example is the effect on the moment of inertia for rotational nuclei, which is always smaller than the rigid-body value at low spin, which can be explained as an effect of pairing correlations. At the same time, the ground states of heavy nuclei with open-shell configurations are reasonably well described by the superfluid Bardeen-Cooper-Schrieffer BCS wave functions with energy gaps of about 1 MeV. Properties of both collective and non-collective (quasiparticle) excitations depend on size of the energy gap. Furthermore, it has been argued by Bertsch [6] that nuclear shape change may be associated with the hopping of nucleon pairs by means of the pairing force. In this case, the

pairing interaction and level crossings play an essential role to determine the collective mass (“hopping mass”).

According to these considerations, the pairing interaction should play a key role in understanding the large amplitude collective motion in nuclei, especially when level crossings are involved as the shape change is taking place. Therefore, it is important to investigate the applicability of ALACM for such a system with level crossings and a pairing force. The theory has not been applied to such systems before.

In this paper, we study a model Hamiltonian describing a system interacting through the pairing force. The model has a single-particle level crossing and multiple local minima, and thus may be regarded as a model for shape-coexistence phenomena. In Sec. II, the formalism of ALACM is briefly recapitulated. In order to apply the ALACM to a classical Hamiltonian with a spurious component (Nambu-Goldstone mode), a modified version of the local harmonic equations is formulated. The classical Hamiltonian for a pairing Hamiltonian is derived in Sec. III, both by using the mean-field (in this case BCS) theory and by applying a parametrisation which exactly conserves particle number. The results of numerical calculations for a simple two-level system are given in Sec. IV and the conclusions and an outlook are summarised in Sec. V.

## II. BRIEF REVIEW OF ALACM

### A. Local harmonic equations (LHE)

We briefly review the theory of ALACM (see Ref. [1] for a complete description). In this section, we use a summation convention where the repeated appearance of the same symbols ( $\alpha, \beta, \dots; i, j, \dots$ ) in upper and lower indices denotes a sum over that symbol for all possible values. We also use the convention that a comma in a lower index indicates the derivative with respect to the coordinate, thus  $F_{,\alpha} = \partial F / \partial \xi^\alpha$ .

The theory of adiabatic large amplitude collective motion (ALACM) is applicable to a classical Hamiltonian system which has kinetic terms only quadratic in momentum. We thus have to start with a truncated Hamiltonian

$$\mathcal{H}(\xi, \pi) = \frac{1}{2} B^{\alpha\beta} \pi_\alpha \pi_\beta + V(\xi) , \quad \alpha, \beta = 1, \dots, n , \quad (2.1)$$

where the mass tensor  $B^{\alpha\beta}$ , in general, depends on the coordinates  $\xi^\alpha$  and is defined by truncation of the Hamiltonian to second order

$$B^{\alpha\beta} = \left. \frac{\partial^2 \mathcal{H}}{\partial \pi_\alpha \partial \pi_\beta} \right|_{\pi=0} . \quad (2.2)$$

Thus all terms more than quadratic in momentum are neglected. In the sense that the higher-order terms are small, this theory may be regarded as an *adiabatic* theory in the small-velocity limit. The tensor  $B_{\alpha\beta}$ , which is defined as the inverse of  $B^{\alpha\beta}$  ( $B^{\alpha\gamma} B_{\gamma\beta} = \delta^\alpha_\beta$ ), plays the role of metric tensor in the Riemannian formulation of local harmonic equations (LHE) below.

Collective coordinates  $q^i$  and intrinsic (non-collective) coordinates  $q^a$  which are approximately decoupled from each other, are assumed to be obtainable by making a point transformation, conserving the quadratic nature of Eq.(2.1),

$$q^i = f^i(\xi) \quad (i = 1, \dots, K) , \quad (2.3)$$

$$q^a = f^a(\xi) \quad (a = K + 1, \dots, n) . \quad (2.4)$$

In this section, we use symbols  $(\alpha, \beta, \dots)$  for indices of original coordinates,  $(\mu, \nu, \dots)$  for new coordinates after the transformation,  $(i, j, \dots)$  for collective coordinates and  $(a, b, \dots)$  for intrinsic coordinates. The new Hamiltonian after the point transformations takes the form,

$$\bar{\mathcal{H}} \approx \frac{1}{2} \bar{B}^{ij} p_i p_j + \frac{1}{2} \bar{B}^{ab} p_a p_b + \bar{V}(q^i, q^a) , \quad (2.5)$$

where we have used the fact that for decoupled motion the mass tensor must be block-diagonal,

$$\bar{B}^{ai} = 0 . \quad (2.6)$$

Besides the block-diagonality of mass tensor, we require the absence of both “real” and “geometrical” forces orthogonal to the decoupled manifold,

$$\bar{V}_{,a} = 0 , \quad (2.7)$$

$$\bar{B}^{ij}_{,a} = 0 . \quad (2.8)$$

In practice, these three decoupling conditions, (2.6), (2.7) and (2.8), cannot be satisfied exactly, except for special cases. Thus, we need a method applicable to an approximately decoupled manifold. The Riemannian formulation of LHE [1] is the one we choose to use in this paper. In a case of a single collective coordinate ( $K = 1$ ), the basic equations of this formalism can be written as

$$V_{,\alpha} = \lambda f_{,\alpha}^1 , \quad (2.9)$$

$$B^{\beta\gamma} V_{;\alpha\gamma} f_{,\beta}^1 = \omega^2 f_{,\alpha}^1 . \quad (2.10)$$

Here the covariant derivative (denoted by  $;$ ) in the l.h.s. of Eq.(2.10) is defined by

$$V_{;\alpha\beta} \equiv V_{,\alpha\beta} - \Gamma_{\alpha\beta}^{\gamma} V_{,\gamma} , \quad (2.11)$$

where the affine connection  $\Gamma$  is defined with the help of metric tensor  $B_{\alpha\beta}$  as

$$\Gamma_{\beta\gamma}^{\alpha} = \frac{1}{2} B^{\alpha\delta} (B_{\delta\beta,\gamma} + B_{\delta\gamma,\beta} - B_{\beta\gamma,\delta}) . \quad (2.12)$$

The equations (2.9) and (2.10) can be solved iteratively, starting from a stationary point. In principle, the procedure to find a collective path is to find successive points at which an eigenvector  $f_{,\alpha}^1$  of the covariant RPA equation (2.10) satisfies the force condition (2.9) at the same time.

Once we get a collective path  $\Sigma$  in multi-dimensional configuration space, a collective Hamiltonian is defined by evaluating the Hamiltonian (2.5) on the path  $\Sigma$ ,

$$\bar{\mathcal{H}}_{\text{col}} = \bar{\mathcal{H}}\Big|_{\Sigma, \pi_a=0} \approx \frac{1}{2} \bar{B}^{11} p_1^2 + \bar{V}(q^1) , \quad (2.13)$$

where we assume a single collective coordinate  $K = 1$ .

The quality of decoupling can be measured by comparing two different collective mass parameters that can be calculated in the theory. If we calculate the derivatives  $d\xi^\alpha/dq^1$  in terms of the tangents of the path,

$$\bar{B}_{11} = \frac{d\xi^\alpha}{dq^1} B_{\alpha\beta} \frac{d\xi^\beta}{dq^1} . \quad (2.14)$$

The other mass parameter can be obtained by using the eigenvectors  $f_{,\alpha}^1$  of the covariant RPA equation.

$$\tilde{B}^{11} = f_{,\alpha}^1 B^{\alpha\beta} f_{,\beta}^1 . \quad (2.15)$$

This is equal to  $(\bar{B}_{11})^{-1}$  if the decoupling is exact. Therefore, we define the decoupling measure  $D$  as

$$D = \left( \bar{B}_{11} \right)^{-1} \tilde{B}^{11} - 1 . \quad (2.16)$$

The size of this measure  $D$  indicates the badness of decoupling.

If the decoupling is good, the motion orthogonal to  $\Sigma$  (motion in directions of  $q^a$ ) becomes irrelevant in classical systems. However, it is not necessarily the case in quantum systems, because, according to the uncertain relation principle, we cannot require  $q_a = 0$  (the motion is confined on  $\Sigma$ ) and  $\pi_a = 0$  at the same time. Therefore, one may need to include the energy correction into the potential  $\bar{V}(q)$ , which arises from quantum fluctuation with respect to the intrinsic degrees of freedom [3]. Subsequently, the collective Hamiltonian  $\bar{\mathcal{H}}_{\text{col}}$  will be quantised in a flat space ( $\bar{B}^{11} = 1$ ) to obtain physical quantities, such as energies and wave functions.

## B. Constrained local harmonic equations (CLHE)

The most practical and straightforward way to investigate a pairing Hamiltonian would be to utilise the mean-field (BCS) approximation (Sec. III A) in which the general product wave functions are no longer eigenstates of the particle number. When an intrinsic ground state breaks a (continuous) symmetry of Hamiltonian, generally speaking, a Nambu-Goldstone (NG) mode will appear. This mode corresponds to an “excitation” to connect degenerate vacua. In the case of particle-number breaking, this is often called “pairing rotation”. We are interested in finding a collective coordinate orthogonal to this trivial mode.

It is also well-known that, at equilibrium points, the NG mode has zero excitation energy and is decoupled from the other modes in the RPA order. Thus, one may easily separate this mode from the other physical modes (unless the physical mode happens to be zero

energy). However, the NG mode does not necessarily have zero energy at non-equilibrium points. Since we have to solve the LHE at each point on the collective path, it is not trivial to distinguish the NG mode from the other modes. Therefore, in this section, we provide a modified formulation of LHE which fixes a value of the coordinate corresponding to the NG mode. In the BCS parametrisation, we need the constraints to fix the particle number and gauge angle (Sec. III A). We shall make use of the fact that the coordinate and momenta corresponding to the NG mode are explicitly known.

We shall only discuss the case of a single collective coordinate  $K = 1$  and a single NG mode. First we divide the set  $\{q^\mu\}$  into three subsets,  $q^1$ ,  $q^{\text{NG}}$ , and  $q^a$ ,  $a = 3, \dots, n$ , which are assumed to be obtained by point transformations

$$q^\mu = f^\mu(\xi) , \quad \xi^\alpha = g^\alpha(q) , \quad (2.17)$$

$$p_\mu = g_{,\mu}^\alpha \pi_\alpha , \quad \pi_\alpha = f_{,\alpha}^\mu p_\mu . \quad (2.18)$$

$q^{\text{NG}}$  represents a coordinate for a NG mode and  $q^1$  for a collective coordinate now we are trying to determine. In the case that the translational symmetry is broken,  $q^{\text{NG}}$  and  $p_{\text{NG}}$  would be the centre-of-mass coordinate and the total momentum, respectively. In the case of particle-number breaking, they correspond to the particle number and the gauge angle. In all these cases we know the explicit form of the coordinates and momenta for the NG mode(s). Thus, we can write  $q^{\text{NG}}$  and  $p_{\text{NG}}$  as functions of original coordinates  $\xi^\alpha$  and momenta  $\pi_\alpha$ . Although in general  $q^{\text{NG}}$  and  $p_{\text{NG}}$  have arbitrary dependence on  $\xi$  and  $\pi$ , we expand them with respect to  $\pi$  up to the zero-th order for  $q^{\text{NG}}$  and up to first order for  $p_{\text{NG}}$ . In keeping with the adiabatic character of the theory, then, we get  $f^{\text{NG}}(\xi^\alpha)$  and  $g_{,\text{NG}}^\alpha(f^\mu(\xi))$ . An example will be shown in the next section for the particle number and the gauge angle.

The conditions for decoupling are again given by three equations (2.6), (2.7) and (2.8), where  $i = 1$  and NG. In this section we use symbols  $(i, j, \dots)$  representing 1 and NG. In Ref. [1] it is shown that the third decoupling condition (2.8) implies that the decoupled surface is a geodesic. The geodesic surface is defined by differential equations

$$g_{,ij}^\alpha + \Gamma_{\beta\gamma}^\alpha g_{,i}^\beta g_{,j}^\gamma - \bar{\Gamma}_{ij}^k g_{,k}^\alpha = 0 , \quad (2.19)$$

$$f_{,\alpha\beta}^i - \Gamma_{\alpha\beta}^\gamma f_{,\gamma}^i + \bar{\Gamma}_{jk}^i f_{,\alpha}^j f_{,\beta}^k = 0 , \quad (2.20)$$

where the affine connection  $\Gamma$  is defined by Eq.(2.12) and  $\bar{\Gamma}$  in new coordinates is in the same manner

$$\bar{\Gamma}_{\mu\nu}^\lambda = \frac{1}{2} \bar{B}^{\lambda\kappa} \left( \bar{B}_{\kappa\mu,\nu} + \bar{B}_{\kappa\nu,\mu} - \bar{B}_{\mu\nu,\kappa} \right) . \quad (2.21)$$

Now we consider constraints

$$q^{\text{NG}} = f^{\text{NG}}(\xi^\alpha) = q_0^{\text{NG}} \quad (= \text{const.}) , \quad (2.22)$$

$$p_{\text{NG}} = g_{,\text{NG}}^\alpha \pi_\alpha = 0 , \quad (2.23)$$

which freeze the NG degree of freedom. The Poisson bracket between these two constraints is  $\{q^{\text{NG}}, p_{\text{NG}}\}_{\text{PB}} = f_{,\alpha}^{\text{NG}} g_{,\text{NG}}^\alpha = 1$ . In order to facilitate the calculation of differentiation, we need to define a Dirac bracket [7] by

$$\{F, G\}_{\text{DB}} \equiv \{F, G\}_{\text{PB}} + \{F, q^{\text{NG}}\}_{\text{PB}} \{p_{\text{NG}}, G\}_{\text{PB}} - \{F, p_{\text{NG}}\}_{\text{PB}} \{q^{\text{NG}}, G\}_{\text{PB}} . \quad (2.24)$$

First we consider the force condition corresponding to Eq.(2.9). We differentiate the potential  $V(\xi) = \bar{V}(q)$  with respect to  $\xi^\alpha$  keeping the constraints  $q^{\text{NG}} = q_0^{\text{NG}}$  and  $p_{\text{NG}} = 0$ .

$$\left. \frac{\partial V}{\partial \xi^\alpha} \right|_{q^{\text{NG}}=q_0^{\text{NG}}} = \bar{V}_{,1} f_{,\alpha}^1 + \bar{V}_{,a} f_{,\alpha}^a = \bar{V}_{,1} f_{,\alpha}^1, \quad (2.25)$$

where the decoupling condition (2.7) has been used. This can be calculated by using the Dirac bracket as

$$\begin{aligned} \left. \frac{\partial V}{\partial \xi^\alpha} \right|_{q^{\text{NG}}=q_0^{\text{NG}}} &= -\{\pi_\alpha, V\}_{\text{DB}}, \\ &= V_{,\alpha} - f_{,\alpha}^{\text{NG}} g_{,\text{NG}}^\beta V_{,\beta}. \end{aligned} \quad (2.26)$$

Equating the above two equations, we obtain the force condition

$$V_{,\alpha} = \bar{V}_{,i} f_{,\alpha}^i. \quad (2.27)$$

In the case of pairing rotation,  $f^{\text{NG}}$  may be taken as the average particle number  $\mathcal{N} \equiv \langle \hat{N} \rangle$ . Then,  $\bar{V}_{,\text{NG}} = \partial V / \partial N$  can be regarded as a chemical potential  $\mu$  and Eq.(2.27) may be rewritten in the form similar to the constrained Hartree-Fock-Bogoliubov equation

$$V_{,\alpha} = \mu \mathcal{N}_{,\alpha} + \lambda f_{,\alpha}^1. \quad (2.28)$$

In order to obtain the covariant RPA equation corresponding to Eq.(2.10), we start with the contravariant derivative of the potential

$$\bar{V}^{,1} = V^{,\beta} f_{,\beta}^1, \quad (2.29)$$

where  $V^{,\alpha} \equiv B^{\alpha\beta} V_{,\beta}$  and  $\bar{V}^{,1} \equiv \bar{B}^{1\mu} \bar{V}_{,\mu} = \bar{B}^{1i} \bar{V}_{,i}$ . Again we differentiate this equation with respect to  $\xi^\alpha$  in keeping with  $q^{\text{NG}} = p_{\text{NG}} = 0$ . The derivative of the l.h.s. is easily calculated as

$$\left. \frac{\partial \bar{V}^{,1}}{\partial \xi^\alpha} \right|_{q^{\text{NG}}=0} = \bar{V}_{,1}^1 f_{,\alpha}^1. \quad (2.30)$$

The derivative of the r.h.s. is calculated in terms of the Dirac bracket.

$$\left. \frac{\partial}{\partial \xi^\alpha} V^{,\beta} f_{,\beta}^1 \right|_{q^{\text{NG}}=0} = -\{\pi_\alpha, V^{,\beta} f_{,\beta}^1\}_{\text{DB}}, \quad (2.31)$$

$$= (V_{,\alpha}^{,\beta} - f_{,\alpha}^{\text{NG}} g_{\text{NG}}^\gamma V_{,\gamma}^{,\beta}) f_{,\beta}^1 + V^{,\beta} (f_{,\alpha\beta}^1 - f_{,\alpha}^{\text{NG}} g_{\text{NG}}^\gamma f_{,\beta\gamma}^1), \quad (2.32)$$

$$= (V_{,\alpha}^{,\beta} - f_{,\alpha}^{\text{NG}} g_{\text{NG}}^\gamma V_{,\gamma}^{,\beta}) f_{,\beta}^1 - \bar{\Gamma}_{i1}^1 \bar{V}^{,i} f_{,\alpha}^1, \quad (2.33)$$

where, from the second to the third lines, we used the geodesic equation (2.20) and the covariant derivative defined by

$$V_{;\alpha}^{,\beta} \equiv V_{,\alpha}^{,\beta} + \Gamma_{\alpha\gamma}^\beta V^{,\gamma}. \quad (2.34)$$

From Eqs.(2.30) and (2.33), we obtain

$$\left(V_{;\alpha}^{\beta} - f_{,\alpha}^{\text{NG}} g_{\text{NG}}^{\gamma} V_{;\gamma}^{\beta}\right) f_{,\beta}^1 = \bar{V}_{;1}^1 f_{,\alpha}^1 . \quad (2.35)$$

Replacing  $\bar{V}_{;1}^1$  by  $\omega^2$ , this becomes the covariant RPA equation to determine eigenfrequencies  $\omega$  and eigenvectors  $f_{,\alpha}^1$ . It is worth noting that any solution  $f_{,\alpha}^1$  of Eq.(2.35) with non-zero eigenfrequency is orthogonal to the NG mode. This may be understood as follows: One multiplies Eq.(2.35) by  $g_{,\text{NG}}^{\alpha}$  and takes sum over  $\alpha$ . Then, since the l.h.s. becomes  $\bar{V}_{,\text{NG}}^1 - \bar{V}_{,\text{NG}}^1 = 0$ , it results in

$$\omega^2 g_{,\text{NG}}^{\alpha} f_{,\alpha}^1 = 0 . \quad (2.36)$$

Therefore, with  $\omega \neq 0$ , we have  $g_{,\text{NG}}^{\alpha} f_{,\alpha}^1 = 0$ .

Since the NG mode emerges only when we break a symmetry of Hamiltonian, one may expect that the CLHE formalism should become the usual LHE when the underlying symmetry is unbroken. In the next section, we will discuss the BCS approximation to derive a classical Hamiltonian system. In the parametrisation of Eq. (3.17) and (3.18), a state with  $|\xi^{\alpha}| = 1$  and  $\pi = 0$  corresponds to a state in a normal phase which is an eigenstate of particle number (from Eq.(3.23), one can see the pairing gap vanish in this case). Then, from Eq.(3.25), we have  $f_{,\alpha}^{\text{NG}} = 0$ . Therefore, the CLHE (2.27) and (2.35) become equivalent to the LHE (2.9) and (2.10).

The equations (2.27) and (2.35) are the defining equations of CLHE formalism. As in the usual LHE, we require the self-consistency between these two equations: A solution of Eq.(2.35) should satisfies Eq.(2.27) at the same time. In this paper, where we concentrate on a simple model, it is easier to solve the constraints  $q^{\text{NG}} = q_0^{\text{NG}}$  and  $p_{\text{NG}} = 0$  explicitly and describe everything by independent canonical variables  $(\xi^{*\alpha}, \pi_{\alpha}^*)$  ( $\alpha = 1, \dots, n-1$ ). However, in the realistic cases for which it is difficult to solve the constraints, this CLHE formalism would become more useful.

### III. TRANSCRIPTION INTO CLASSICAL FORM

We consider a simple model where particles coupled to a harmonic oscillator interact through the pairing force, first introduced by Fukui, Matsuo and Matsuyanagi [8] in order to study shape mixing. This model can be regarded as a vibrating core plus valence particles which can move between different levels by the pairing force,

$$H = H_{\text{core}} + H_{\text{val}} , \quad (3.1)$$

where

$$H_{\text{core}} = \frac{1}{2} (p^2 + q^2) , \quad (3.2)$$

$$H_{\text{val}} = \sum_{\alpha=1}^{\Omega} \epsilon_{\alpha}(q) \left( c_{\alpha}^{\dagger} c_{\alpha} + c_{\bar{\alpha}}^{\dagger} c_{\bar{\alpha}} \right) - G \hat{P}^{\dagger} \hat{P} , \quad (3.3)$$

and we assume  $G > 0$ . Here  $\bar{\alpha}$  denotes the time-reversed state of  $\alpha$  and  $\hat{P}^{\dagger} = \sum_{\alpha>0} c_{\alpha}^{\dagger} c_{\bar{\alpha}}^{\dagger}$  is the pair creation operator. The total number of levels is  $2\Omega$ . The single-particle energies  $\epsilon_{\alpha}(q)$  depend on the “deformation”  $q$  of the core, which induces particle-core coupling.



We need to construct a classical Hamiltonian which describes the dynamics of the valence particles. In order to do this, time-dependent mean-field theory, which is known to be a form of Hamilton's equation, is utilised in the next section. This is of practical interest because it has applicability to realistic systems. For the current model one can also adopt a direct parametrisation of the exact wave function to construct a classical Hamiltonian (Sec. III B).

### A. The time-dependent mean-field (TDMF) equation

In this section we describe a canonical parametrisation of a general product wave function, discussed in Ref. [9]. We start with a BCS state  $|\phi_0\rangle$  which is the vacuum to quasiparticle operators  $a_\alpha$ ,

$$a_\alpha^\dagger = u_\alpha c_\alpha^\dagger - v_\alpha c_{\bar{\alpha}} , \quad (3.4)$$

$$a_{\bar{\alpha}}^\dagger = u_\alpha c_{\bar{\alpha}}^\dagger + v_\alpha c_\alpha . \quad (3.5)$$

According to Thouless' theorem [10], any other general product wave function  $|z\rangle$  which is not orthogonal to  $|\phi_0\rangle$  may be written in the form

$$|z\rangle = \exp \left\{ \frac{1}{2} \sum_{\alpha\beta} z_{\alpha\beta} a_\alpha^\dagger a_\beta^\dagger \right\} |\phi_0\rangle , \quad (3.6)$$

where  $z_{\alpha\beta} = -z_{\beta\alpha}$ .

The time-dependent BCS equation can be obtained by taking variations with respect to  $z$  and  $z^*$  of the classical action,

$$S = \int_{t_i}^{t_f} dt \frac{\langle z | i\partial_t - H | z \rangle}{\langle z | z \rangle} . \quad (3.7)$$

We can introduce canonical coordinates  $(\xi_{\alpha\beta}, \pi_{\alpha\beta})$  by  $\beta_{\alpha\beta} = (\xi_{\alpha\beta} + i\pi_{\alpha\beta})/\sqrt{2}$ , for  $\alpha > \beta$ . For  $\alpha < \beta$  antisymmetry tells us that the same coordinates are involved,

$$\beta_{\alpha\beta} = -\beta_{\beta\alpha} = (\xi_{\beta\alpha} + i\pi_{\beta\alpha})/\sqrt{2} \quad (3.8)$$

we can easily relate  $\beta$  and  $z$  by

$$\beta_{\alpha\beta} = \left[ z(1 + z^\dagger z)^{-1/2} \right]_{\alpha\beta} . \quad (3.9)$$

This means that *quasi*-density matrices and *quasi*-pairing tensors can be expressed by

$$\bar{\rho}_{\alpha\gamma} = \frac{\langle z | a_\gamma^\dagger a_\alpha | z \rangle}{\langle z | z \rangle} = [\beta \beta^\dagger]_{\alpha\gamma} , \quad (3.10)$$

$$\bar{\kappa}_{\alpha\gamma} = \frac{\langle z | a_\gamma a_\alpha | z \rangle}{\langle z | z \rangle} = [\beta(1 - \beta^\dagger \beta)^{1/2}]_{\alpha\gamma} . \quad (3.11)$$

Using Eqs.(3.4) and (3.5), one can relate these quantities with *real* density matrices  $\rho_{\alpha\gamma} = \langle c_\gamma^\dagger c_\alpha \rangle$  and pairing tensors  $\kappa_{\alpha\gamma} = \langle c_\gamma c_\alpha \rangle$ .

Then, the equations of motion take the canonical form (using an implicit matrix notation)

$$\dot{\xi} = \frac{\partial \mathcal{H}}{\partial \pi} , \quad (3.12)$$

$$\dot{\pi} = -\frac{\partial \mathcal{H}}{\partial \xi} , \quad (3.13)$$

with a classical Hamiltonian

$$\mathcal{H}(\xi, \pi) = \frac{\langle z|H|z \rangle}{\langle z|z \rangle} . \quad (3.14)$$

Since monopole pairing interactions in nuclei were originally introduced in order to give a simple model of the short-range attractive force, often only the Hartree terms are taken into account in the mean-field calculations. Thus, we shall neglect the exchange terms in Sec. IV A. If we neglect the exchange terms for the Hamiltonian (3.3), only  $(\alpha\gamma) = (\alpha\bar{\alpha})$  components are available and the matrix relations can be regarded as ordinary  $c$ -number relations. For instance, Eqs.(3.10) and (3.11) now take the form

$$\bar{\rho}_{\alpha\bar{\alpha}} = \beta_{\alpha\bar{\alpha}}\beta_{\alpha\bar{\alpha}}^* , \quad \bar{\kappa}_{\alpha\bar{\alpha}} = \beta_{\alpha\bar{\alpha}}(1 - \beta_{\alpha\bar{\alpha}}^*\beta_{\alpha\bar{\alpha}})^{1/2} , \quad (3.15)$$

where there is no summation with respect to the indices  $(\alpha, \bar{\alpha})$ .

The coordinates defined above depend on the reference state  $|\phi_0\rangle$ . For practical applications, it is probably convenient to use a local coordinate at each point on a collective path when one solves the LHE [2]. Namely, when moving to a nearby point, one changes the reference state to the Slater determinant at this new point, making the new point the origin of coordinate system, and solves the LHE. However, in this paper, in order to visualise a collective path in the configuration space, we use a fixed reference state and a global coordinate system. Since this global coordinate system cannot describe a state  $|\phi\rangle$  which is orthogonal to the reference state  $|\phi_0\rangle$ , we need to select a reference state suitable for describing all relevant states.

In case that we consider a system with  $N = \Omega$  particles, we may take the BCS state with  $u_\alpha = v_\alpha = 1/\sqrt{2}$  for all  $\alpha$  as the  $|\phi_0\rangle$  ( $\langle\phi_0|\hat{N}|\phi_0\rangle = \Omega$ ). The classical Hamiltonian for valence particles (3.3) may be written as

$$\begin{aligned} \mathcal{H}_{\text{val}}(\xi, \pi) = \sum_{\alpha>0} \epsilon_\alpha(q) \left[ 1 + \sqrt{2}\xi_\alpha \left\{ 1 - \frac{1}{2}(\xi_\alpha^2 + \pi_\alpha^2) \right\}^{1/2} \right] \\ - \frac{G}{4} \left[ (\Omega - \xi^2 - \pi^2)^2 + 2 \left\{ \sum_{\alpha>0} \pi_\alpha \left( 1 - \frac{1}{2}(\xi_\alpha^2 + \pi_\alpha^2) \right)^{1/2} \right\}^2 \right] , \end{aligned} \quad (3.16)$$

where we used notations  $\xi_\alpha \equiv \xi_{\alpha\bar{\alpha}}$ ,  $\pi_\alpha \equiv \pi_{\alpha\bar{\alpha}}$ ,  $\xi^2 \equiv \sum_\alpha \xi_\alpha^2$ ,  $\pi^2 \equiv \sum_\alpha \pi_\alpha^2$ , and neglected the exchange terms. Expanding this Hamiltonian up to second order in momentum, we obtain an adiabatic Hamiltonian in the form of Eq.(2.1) with

$$B^{\alpha\beta}(\xi) = \frac{\partial^2 \mathcal{H}_{\text{val}}}{\partial \pi_\alpha \partial \pi_\beta} \Big|_{\pi=0} = \left\{ -\frac{\epsilon_\alpha(q)}{\sqrt{2}} \frac{\xi_\alpha}{\Xi_\alpha} + G(\Omega - \xi^2) \right\} \delta_{\alpha\beta} - G\Xi_\alpha \Xi_\beta , \quad (3.17)$$

$$V(\xi) = \mathcal{H}_{\text{val}}(\xi, \pi = 0) = \sqrt{2} \sum_{\alpha>0} \epsilon_\alpha(q) \xi_\alpha \Xi_\alpha - \frac{G}{4} (\Omega - \xi^2)^2 , \quad (3.18)$$

where

$$\Xi_\alpha = \left(1 - \frac{1}{2}\xi_\alpha^2\right)^{1/2}, \quad (3.19)$$

The average number of particles is

$$\mathcal{N}(\xi, \pi) = \frac{\langle z | \hat{N} | z \rangle}{\langle z | z \rangle} = \Omega + \sqrt{2} \sum_{\alpha>0} \xi_\alpha \left\{ 1 - \frac{1}{2}(\xi_\alpha^2 + \pi_\alpha^2) \right\}^{1/2}, \quad (3.20)$$

$$\approx \Omega + \sqrt{2} \sum_{\alpha>0} \xi_\alpha \Xi_\alpha + O(\pi^2). \quad (3.21)$$

The pairing gap is

$$\Delta(\xi, \pi) = G \frac{\langle z | \hat{P} | z \rangle}{\langle z | z \rangle} = \frac{G}{2} \left[ \Omega - \xi^2 - \pi^2 + \sqrt{2}i \sum_{\alpha>0} \pi_\alpha \left\{ 1 - \frac{1}{2}(\xi_\alpha^2 + \pi_\alpha^2) \right\}^{1/2} \right], \quad (3.22)$$

$$\approx \frac{G}{2} \left\{ \Omega - \xi^2 + \sqrt{2}i \sum_{\alpha>0} \pi_\alpha \Xi_\alpha \right\} + O(\pi^2). \quad (3.23)$$

Thus, the gauge angle  $\varphi$  in the adiabatic limit can be expressed by

$$\varphi = \arctan \frac{\text{Im}\Delta}{\text{Re}\Delta} \approx \frac{\sqrt{2}}{\Omega - \xi^2} \sum_{\alpha>0} \pi_\alpha \Xi_\alpha + O(\pi^3). \quad (3.24)$$

Since we consider a system with  $N = \Omega$  particles, we may regard  $(\mathcal{N} - \Omega)/2$  as  $q^{\text{NG}}$  and  $\varphi$  as  $p_{\text{NG}}$  in Sec. II B. Using the adiabatic expression of the particle number (3.21) and the gauge angle (3.24), we can identify

$$f^{\text{NG}}(\xi) = \frac{\mathcal{N}^{\text{ad}} - \Omega}{2} = \frac{1}{\sqrt{2}} \sum_{\alpha>0} \xi_\alpha \Xi_\alpha, \quad (3.25)$$

$$\frac{\partial g^\alpha}{\partial q^{\text{NG}}}(\xi) = \frac{\partial \varphi}{\partial \pi_\alpha} \Big|_{\pi=0} = \frac{\sqrt{2}}{\Omega - \xi^2} \Xi_\alpha. \quad (3.26)$$

One can see that the canonical relation

$$\left\{ \frac{\mathcal{N}^{\text{ad}}}{2}, \varphi^{\text{ad}} \right\}_{\text{PB}} = \sum_\alpha \frac{\partial f^{\text{NG}}}{\partial \xi_\alpha} \frac{\partial g^\alpha}{\partial q^{\text{NG}}} = 1, \quad (3.27)$$

is satisfied.

In case of  $N = \Omega = 2$ , the conservation of particle number in the adiabatic limit (3.21) is simply satisfied by

$$\xi_1 = -\xi_2, \quad \pi_1 = -\pi_2. \quad (3.28)$$

Then,  $\mathcal{H}_{\text{val}}$  can be expressed as

$$\mathcal{H}_{\text{val}} = \frac{1}{2} B^{\text{val}} \pi^2 + V(\xi), \quad (3.29)$$

$$B_{\text{val}} = -\frac{\sqrt{2}\epsilon\xi}{4\Xi} + G(1 - \xi^2), \quad (3.30)$$

$$V(\xi) = 2\sqrt{2}\epsilon\xi\Xi - G(1 - \xi^2)^2, \quad (3.31)$$

where we assume  $\epsilon \equiv \epsilon_1 = -\epsilon_2$  and

$$\xi \equiv \xi_1 = -\xi_2, \quad \pi \equiv \pi_1 - \pi_2 = 2\pi_1, \quad \Xi \equiv \left(1 - \frac{1}{2}\xi^2\right)^{1/2}. \quad (3.32)$$

The potential is stationary at

$$\xi = \pm 1, \quad (3.33)$$

$$\text{and } -\frac{\text{sgn}\epsilon}{\sqrt{2}} \left( \sqrt{1 + \frac{|\epsilon|}{G}} \pm \sqrt{1 - \frac{|\epsilon|}{G}} \right), \text{ for } |\epsilon| < G. \quad (3.34)$$

At  $\xi = 1$  ( $-1$ ) two particles occupy the  $\alpha = 1$  ( $\alpha = 2$ ) level. For  $\epsilon \neq 0$ , one of the states corresponds to a local minimum and the other to a local maximum. For  $|\epsilon| < G$ , the potential has another local minimum which corresponds to a superfluid state (the upper and lower signs in Eq.(3.34) give the same state in the limit of  $\pi = 0$ ).

### B. The time-dependent Schrödinger equation (TDSE)

In case of  $N = \Omega = 2$ , one can easily find a canonical parametrisation for the exact time-dependent Schrödinger equation (TDSE). With a notation  $|\alpha\bar{\alpha}\rangle = c_\alpha^\dagger c_{\bar{\alpha}}^\dagger |0\rangle$ , normalised states can be written in general as

$$|\psi(t)\rangle = e^{i\phi(t)} \cos(\alpha(t)) |1\bar{1}\rangle + e^{-i\phi(t)} \sin(\alpha(t)) |2\bar{2}\rangle. \quad (3.35)$$

An action, similar to Eq.(3.7), may be defined by

$$S = \int_{t_i}^{t_f} dt \langle \psi(t) | i\partial_t - H | \psi(t) \rangle. \quad (3.36)$$

The time-dependent Schrödinger equation can be given in terms of the least action principle. For the Hamiltonian  $H_{\text{val}}$ , we can introduce canonical coordinates  $(\xi, \rho)^1$  as follows.

$$\xi = \alpha, \quad \rho = -2\phi \sin 2\alpha. \quad (3.37)$$

The canonical equations of motion (3.12) and (3.12) hold for the Hamiltonian

$$\mathcal{H}_{\text{val}} = \langle \psi | H_{\text{val}} | \psi \rangle = 2\epsilon \cos 2\xi - G \left\{ 1 + \sin 2\xi \cos \left( -\frac{\rho}{\sin 2\xi} \right) \right\}, \quad (3.38)$$

where  $\epsilon \equiv \epsilon_1 = -\epsilon_2$ . The adiabatic Hamiltonian (3.29) is obtained by expanding up to second order in momentum. The resultant mass parameter and potential are

$$B_{\text{val}}(\xi) = \frac{G}{\sin 2\xi}, \quad (3.39)$$

$$V(\xi) = 2\epsilon \cos 2\xi - G(1 + \sin 2\xi). \quad (3.40)$$

---

<sup>1</sup> In order to avoid confusion with  $\pi = 3.14\dots$ , in this section we use the symbol  $\rho$  for the momentum conjugate to  $\xi$ .

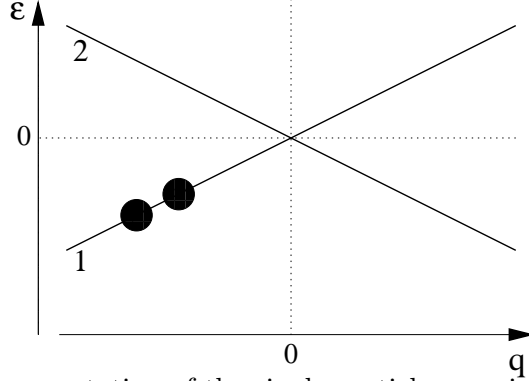


FIG. 1. A schematic representation of the single-particle energies as a function of the coordinate  $q$ , for the case  $\epsilon_0 = 0$ ,  $\chi > 0$ .

In this parametrisation, the mass does not depend on the single-particle energy  $\epsilon$ . It is apparent from Eq.(3.35) that  $\xi = 0$  ( $\pi/2$ ) corresponds to a pure configuration  $|1\bar{1}\rangle$  ( $|2\bar{2}\rangle$ ). There are two stationary points of the potential in a region  $0 \leq \xi \leq \pi$  which are specified by a condition

$$\tan 2\xi = \tan 2\alpha = -\frac{G}{2\epsilon}. \quad (3.41)$$

These give eigenstates (3.35) of  $H_{\text{val}}$  with  $\phi = 0$ . For  $G \geq 0$ , the state in a region  $0 \leq \xi \leq \pi/2$  always has lower energy and the mass parameter  $B_{\text{val}}$  is non-negative in this region.

#### IV. RESULTS

In this section, we present the numerical results for a simple case with  $N = \Omega = 2$ . For single-particle energies, a linear dependence on the coordinate  $q$  is assumed,

$$\epsilon_\alpha(q) = (-)^{\alpha+1}\epsilon(q) = (-)^{\alpha+1}(\chi q - \epsilon_0), \quad \text{for } \alpha = 1, 2. \quad (4.1)$$

The two levels cross each other at  $q = \epsilon_0/\chi$ . A schematic figure of single-particle levels are displayed as functions of  $q$  in Fig. 1. Each level has two-fold degeneracy.

The model can be solved quantum mechanically using a direct product basis  $|N_{\text{osc}}\rangle_{\text{core}} \otimes |\alpha\bar{\alpha}\rangle_{\text{val}}$  where  $|N_{\text{osc}}\rangle_{\text{core}}$  is an eigenstate of the core Hamiltonian with the oscillator quanta  $N_{\text{osc}}$  and  $|\alpha\bar{\alpha}\rangle_{\text{val}} \equiv c_\alpha^\dagger c_{\bar{\alpha}}^\dagger |0\rangle$  ( $\alpha = 1, 2$ ). We use core states with  $N_{\text{osc}} \leq 20$  for diagonalising the total Hamiltonian, which can be written in a matrix form

$$H = \frac{1}{2}(p^2 + q^2)I + \begin{pmatrix} 2\epsilon_1(q) - G & -G \\ -G & 2\epsilon_2(q) - G \end{pmatrix}, \quad (4.2)$$

where  $I$  is the  $2 \times 2$  unit matrix. Results obtained with this method will be referred below as “exact calculation”.

##### A. TDMF parametrisation

Now we apply the theory of ALACM to this model with the mean-field parametrisation in Sec. III A. The Hamiltonian has the form

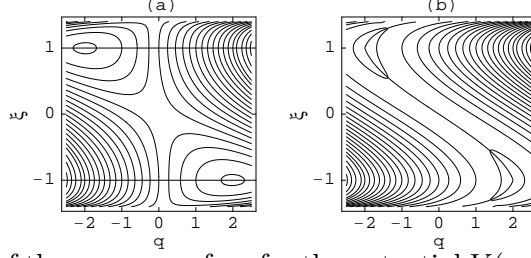


FIG. 2. Contour plots of the energy surface for the potential  $V(q, \xi)$ , Eq.(4.4). The parameters  $\epsilon_0 = 0$  and  $\chi = 1$  are used. The left figure (a) is the energy surface for  $G = 0.2$  and the right (b) for  $G = 1.9$ . Contour lines are displayed for  $\Delta V = 0.5$ . The thick lines indicate the collective paths obtained by the ALACM theory.

$$\mathcal{H} = \frac{1}{2} (p^2 + B_{\text{val}} \pi^2) + V(q, \xi) , \quad (4.3)$$

$$V(q, \xi) = \frac{1}{2} q^2 + 2\sqrt{2}(\chi q - \epsilon_0)\xi\Xi - G(1 - \xi^2)^2 , \quad (4.4)$$

where  $B_{\text{val}}$  is given by Eq.(3.30) with  $\epsilon = \chi q - \epsilon_0$ .

Taking  $\epsilon_0 = 0$  and  $\chi = 1$ , the potential  $V(q, \xi)$  has two local minima at  $(q, \xi) = (-2, 1)$  and  $(2, -1)$  which correspond to valence-particle configurations  $|1\bar{1}\rangle$  and  $|2\bar{2}\rangle$ , respectively. A collective path is now obtained by using the LHE algorithm described in Sec. II. We start from a local minimum, solve the RPA equations and search for the next point in the direction of the lowest RPA mode. Since this system has only two degrees of freedom, we can easily visualise the path on the 2-dimensional surface. In Fig. 2, the potential energy surface and the obtained collective path are shown for two strengths of the pairing force  $G = 0.2$  and  $G = 1.9$ . In the case of  $\epsilon_0 = 0$ , the potential landscape has a symmetry with respect to a rotation of  $180^\circ$  about the origin,  $V(q, \xi) = V(-q, -\xi)$ . For a weak pairing force (Fig. 2 (a)), each local minimum has an independent collective path which represents a harmonic oscillator with a fixed valence configuration (both particles in level 1 or level 2). These represent diabatic solutions which do not mix in this approximation. On the other hand, for a strong pairing force (Fig. 2 (b)), we get a collective path which changes the particle configuration and connects the two local minima.

We have thus found that the system automatically selects different type of collective paths according to the strength of pairing force. In this approximation, we get completely diabatic solutions for  $G = 0.2$  which will result in no parity splitting upon quantisation. Of course, for  $G \neq 0$ , an exact calculation always gives some splitting in energy. However, the splitting turns out to be extremely small for the weak pairing case (see below).

Next, in order to discuss a case of asymmetric potential landscape, let us take  $\epsilon = 0.4$ ,  $\chi = 0.7$  and  $G = 0.1$ . Fig. 3 (a) shows the potential energy surface and collective path. The potential, which is no longer symmetric about the  $180^\circ$  rotation about the origin, has a deep minimum at  $(q, \xi) = (-1.4, 1)$  and a shallow minimum at  $(1.4, -1)$ . Each minimum has again an independent collective path parallel to the horizontal line ( $q$ -axis), representing the diabatic dynamics. In Fig. 3 (b), we show results of exact calculation for this parameter set, together with the diabatic potential curves corresponding to the valence configuration  $|1\bar{1}\rangle$  and  $|2\bar{2}\rangle$ . The number on each level indicates the percentage of the main configuration in the wave function. The exact calculation shows strong diabaticity of the system and two different configurations hardly mix. This agrees with the independent paths obtained in the

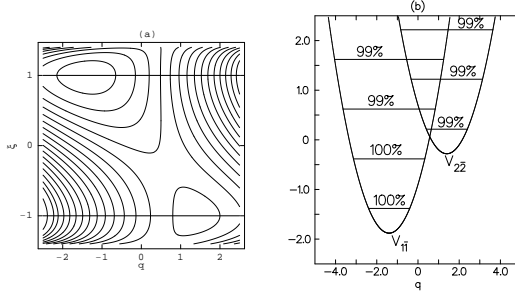


FIG. 3. (a) The same as Fig. 2 but for  $\epsilon = 0.4$ ,  $\chi = 0.7$  and  $G = 0.1$ . (b) Diabatic potential curves as functions of  $q$  and eigenenergies of the exact calculation. The number on each level indicates the percentage of the main configuration in the wave function.

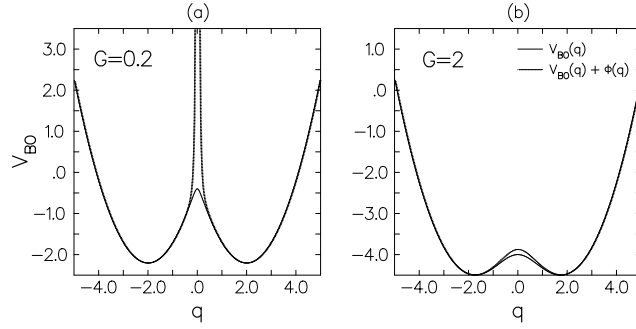


FIG. 4. Born-Oppenheimer potentials  $V(q)$  (solid lines), Eq.(4.6), for  $G = 0.2$  (a) and for  $G = 2$  (b). The parameters  $\epsilon_0 = 0$  and  $\chi = 1$  are used. The dotted lines indicate the potential including the scalar gauge potential,  $V(q) + \Phi(q)$ . See text for details.

ALACM. Therefore, one may state that the ALACM combined with the BCS approximation can reproduce the qualitative feature of the pairing systems.

## B. Born-Oppenheimer (BO) approximation

Before discussing another parametrisation in the next section, let us review the Born-Oppenheimer (BO) approximation. The formulation in the next section can be seen as the generalised version of BO theory, in which a collective coordinate is chosen self-consistently.

Using the conventional adiabatic theory which assumes motion of the valence particles is much faster than motion of the core, the effective Hamiltonian can be obtained by diagonalising  $H_{\text{val}}$  at each value of  $q$ .

$$\bar{H}_{\text{BO}} = \frac{p^2}{2} + V_{\text{BO}}(q), \quad (4.5)$$

$$V_{\text{BO}}(q) = \frac{q^2}{2} - \sqrt{4(\chi q - \epsilon_0)^2 + G^2} - G. \quad (4.6)$$

If we neglect the interaction ( $G = 0$ ), the potential  $V_{\text{BO}}(q)$  has two local minima at  $q = \pm\chi$  corresponding to different valence-particle configurations. Fig. 4 shows the BO potentials  $V_{\text{BO}}(q)$  for weak (Fig. 4 (a)) and strong pairing force (Fig. 4 (b)) with  $\chi = 1$  and  $\epsilon_0 = 0$ . In Ref. [8] it has been shown that this approximation works well for the strong pairing case but it considerably overestimates the mixing between two minima for the weak pairing case.

One possible way to improve the BO theory is to determine a collective path self-consistently and take into account the effect of mass parameter  $B_{\text{val}}$ . This will be discussed in the next section. The other, which is discussed here, is to take account of the (Berry's) "gauge" potentials which emerge from the derivative of the eigenstates of the fast degrees of freedom (valence particles)  $|n\rangle$  with respect to the slow coordinate  $q$ . The new effective Hamiltonian will be

$$\tilde{H}_{\text{BO}} = \frac{1}{2} (p - A_n(q))^2 + V_{\text{BO}}(q) + \Phi_n(q) , \quad (4.7)$$

where

$$A_n(q) \equiv i\langle n | \partial_q n \rangle , \quad (4.8)$$

$$\Phi_n(q) \equiv \frac{1}{2} \langle \partial_q n | (1 - |n\rangle\langle n|) | \partial_q n \rangle . \quad (4.9)$$

In the present case, we take  $|n\rangle$  to be the lowest eigenstate of the valence Hamiltonian which can be expressed as in Eq.(3.35), with  $\alpha$  given by Eq.(3.41). Then, the gauge potentials are calculated as

$$A(q) = 0 , \quad \Phi(q) = \frac{(\chi G)^2}{2 \{4(\chi q - \epsilon_0)^2 + G^2\}^2} . \quad (4.10)$$

This shows that there is no Berry's phase for the current problem, but does imply an additional scalar potential. The additional potential is positive definite and has the maximum value at the crossing point  $q = \epsilon_0/\chi$ . This scalar potential is shown in Fig. 4 by dotted lines. The peak height at a level crossing is getting higher for weaker pairing. This term will suppress the mixing between two minima for the case of weak pairing, and improve the result of quantisation (see below).

### C. TDSE parametrisation

In the Sec. IV A, we have shown the results using the mean-field parametrisation of the valence Hamiltonian, which leads to a diabatic solution in the weak pairing case. In this section, we use the parametrisation described in Sec. III B. This conserves number of particles exactly and can be regarded as a generalised BO theory.

The total Hamiltonian is in a form

$$\mathcal{H} = \frac{1}{2} (p^2 + B_{\text{val}}\pi^2) + V(q, \xi) , \quad (4.11)$$

$$V(q, \xi) = \frac{1}{2} q^2 + 2(\chi q - \epsilon_0) \cos 2\xi - G(1 + \sin 2\xi) , \quad (4.12)$$

where  $B_{\text{val}}$  is given by Eq.(3.39).



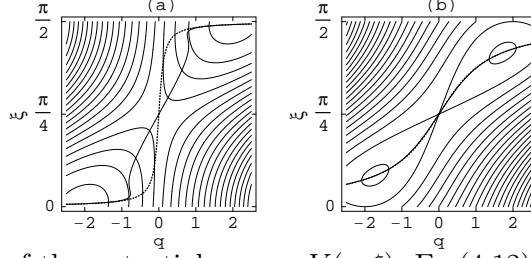


FIG. 5. Contour plots of the potential energy  $V(q, \xi)$ , Eq.(4.12), for  $G = 0.2$  (a) and  $G = 2$  (b). The parameters  $\epsilon_0 = 0$  and  $\chi = 1$  are used. The thick lines indicate the collective paths obtained by the ALACM, while the dotted lines are the paths in the BO approximation.

With  $\epsilon_0 = 0$  and  $\chi = 1$ , the potential surface has again two local minima at

$$(q, \xi) = \left( -\frac{\sqrt{16 - G^2}}{2}, \frac{1}{2} \arccos \left( \frac{\sqrt{16 - G^2}}{4} \right) \right),$$

$$\text{and } \left( \frac{\sqrt{16 - G^2}}{2}, \frac{1}{2} \arccos \left( -\frac{\sqrt{16 - G^2}}{4} \right) \right), \quad (4.13)$$

and a saddle point at  $(0, \pi/4)$  where we restrict  $\xi$  to the region  $0 \leq \xi \leq \pi/2$ . In this parametrisation,  $\xi$  represents the mixing angle between the two valence configurations,  $|1\bar{1}\rangle$  and  $|2\bar{2}\rangle$ . If we minimise the potential with respect to the coordinate  $\xi$  at each value of  $q$ , the potential  $V(q, \xi_0(q))$  becomes the same as the BO potential (4.6). If  $G = 0$ , the local minima correspond to the pure configurations,  $|1\bar{1}\rangle$  ( $\xi = 0$ ) and  $|2\bar{2}\rangle$  ( $\xi = \pi/2$ ). In general, these minima have finite values of mixing angle, which was not the case in the mean-field parametrisation.

Fig. 5 shows the potential energy surfaces and the 1-dimensional collective paths. For a strong pairing force (Fig. 5 (b)), we have a smooth path which connects two local minima. On the other hand, for the case of weak pairing (Fig. 5 (a)), the path exhibits a peculiar kink-like behaviour near  $q = \pm 0.8$ . Close to a local minimum point, the collective path represents a harmonic oscillator (the core Hamiltonian) which is almost parallel to a  $q$ -axis (horizontal line). On the other hand, at the saddle point  $(q, \xi) = (0, \pi/4)$ , the collective path is trying to go through the valley of potential. These paths are not able to be connected smoothly for the weak pairing case, which results in the strange back-bending. In the vicinity of this back-bending, the decoupling from the other degree of freedom is very bad (see discussion below).

In the same figure, we show a path (dotted line) which is obtained by minimising the potential energy at each value of  $q$  (BO approximation). For weak pairing, the path obtained by the ALACM theory is found to be quite different from that by the BO theory. On the other hand, for strong pairing, we can hardly see the difference between them. In the BO approximation, the motion along  $\xi$ -axis is assumed to be much faster than that along  $q$ -axis. In other words, the mass of valence Hamiltonian  $1/B_{\text{val}}$  should be much smaller than the mass of core Hamiltonian, which can be expressed as the condition

$$G \gg \sin 2\xi. \quad (4.14)$$

It is obvious from this equation that the BO approximation fails for the weak pairing force  $G \ll 1$ .

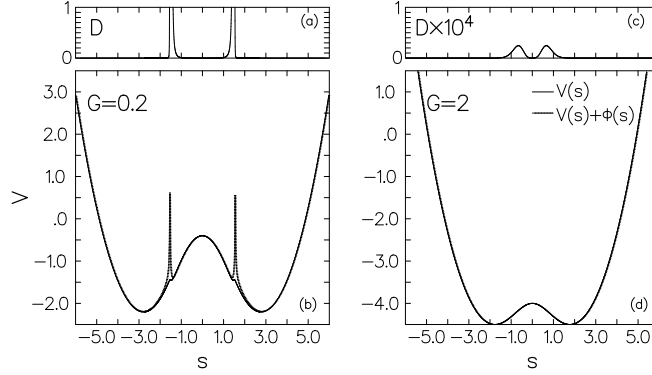


FIG. 6. Potentials along the paths (thick lines) displayed in Fig. 5 as functions of a collective coordinate  $s$  for  $G = 0.2$  (b) and  $G = 2$  (d). Solid (dotted) lines are the potentials without (with) a scalar gauge potential  $\Phi(s)$ . The upper part, (a) and (c), shows the decoupling measure  $D$  defined in Eq.(2.16) for  $G = 0.2$  and  $G = 2$ , respectively.

In order to requantise the obtained collective Hamiltonian, it is convenient to define the collective coordinate  $s$  on the path so as to make the collective mass parameter  $\bar{B}^{11} = 1$ . We use the relation

$$\left(\frac{dq}{ds}\right)^2 + \frac{\sin 2\xi}{G} \left(\frac{d\xi}{ds}\right)^2 = (\bar{B})^{-1} = 1, \quad (4.15)$$

to renormalise the effect of collective mass into a new coordinate  $s$ . The requantised collective Hamiltonian will be in a form

$$\hat{\mathcal{H}} = -\frac{1}{2} \frac{d^2}{ds^2} + \bar{V}(s), \quad (4.16)$$

where  $\bar{V}(s) \equiv V(q(s), \xi(s))$ .

In Fig. 6, the potential and the decoupling measure  $D$  (2.16) are shown as functions of coordinate  $s$ . Comparing these potentials with the BO potentials in Fig. 4, for the strong pairing case, we see that they resemble each other and the decoupling is found to be very good everywhere on the path. For the weak pairing force, however, the distance between two minima of the potential is larger in the ALACM than in the BO theory. The decoupling is extremely bad where the path has a kink (the decoupling measure  $D$  is order of  $10^3$  at the peak), though the decoupling is relatively good anywhere else on the path.

As we have done for the BO approximation, we can incorporate the effective “gauge” potentials into the ALACM theory. We assume gaussian wave functions for the intrinsic (non-collective) degrees of freedom (“harmonic approximation”). Here, collective and intrinsic coordinates are expressed by  $s$  and  $x$ , respectively. The wave function is approximated in a form of semi-direct product,

$$\Psi(s, x) = \psi_{\text{col}}(s) \otimes \psi_{\text{intr}}(s, x), \quad (4.17)$$

where the wave functions for the intrinsic motion  $\psi_{\text{intr}}(s, x)$  are assumed to be a gaussian,

$$\psi_{\text{intr}}(s, x) = \left( \frac{\omega_x(s)}{\pi} \right)^{1/4} \exp \left( -\frac{\omega_x(s)}{2} x^2 \right) . \quad (4.18)$$

Here the frequency  $\omega_x(s)$  are calculated by the covariant RPA at each point on the collective path. Since the lowest RPA mode is supposed to be along the collective path,  $\omega_x(s)$  is the frequency of the second RPA mode.

Identifying  $\psi_{\text{intr}}(s, x)$  with a state  $|n\rangle$  in Eqs.(4.8) and (4.9), the (Berry's) gauge potentials become

$$A(s) \equiv i \int_{-\infty}^{\infty} dx \psi_{\text{intr}}^* \frac{\partial \psi_{\text{intr}}}{\partial s} = 0 , \quad (4.19)$$

$$\Phi(s) \equiv \frac{1}{2} \int_{-\infty}^{\infty} dx \left| \frac{\partial \psi_{\text{intr}}}{\partial s} \right|^2 = \frac{1}{16} \left( \frac{d}{ds} \ln \omega(s) \right)^2 . \quad (4.20)$$

Again, the vector potential  $A$  vanishes and the scalar potential is positive definite. In Fig. 6, we show this scalar gauge potential as a function of  $s$  (dotted lines). For a strong pairing force  $\Phi(s) \approx 0$  everywhere (one cannot see the dotted line in the figure because it almost coincides with the solid line), however, for weak pairing, it has sharp peaks at kinks where the decoupling measure  $D$  also has large values. The requantised Hamiltonian (4.16) will be modified into

$$\hat{\mathcal{H}} = -\frac{1}{2} \frac{d^2}{ds^2} + \bar{V}(s) + \Phi(s) . \quad (4.21)$$

The wave function  $\psi_{\text{col}}(s)$  in Eq.(4.17) is required to be an eigenfunction of this modified Hamiltonian.

The results after requantisation are summarised in Fig. 7. There we show the spectra of (1) the BO theory without gauge potentials, (2) the BO theory with gauge potentials, (3) the ALACM theory without gauge potentials, (4) the ALACM theory with gauge potentials, and (5) the exact calculation. For a strong pairing force, all approximation schemes work well. On the other hand, for a weak pairing force, the result (1) overestimates the splitting of parity doublets. This overestimate is corrected by including the scalar gauge potential (2). The same effect also appears for ALACM results (3) and (4). However, in this case, the suppression of parity splitting originates in the mass parameter, not in the gauge potentials. Since we renormalise the mass parameter with Eq.(4.15), this produces a larger distance between two local minima of the potential  $\bar{V}(s)$ , as compared to  $V_{\text{BO}}(q)$ . The tunnelling probability between two minima is suppressed by this mass-renormalisation effect. The effect of gauge potentials, the difference between (3) and (4), turns out not to be significant in the ALACM. The agreement with the exact calculation is good for low-lying states (up to the third excited state), though, as expected, it is not so good for higher-lying states.

We also show transition matrix elements  $|\langle n'|q|n\rangle|$  in the same figure. They are calculated by

$$\langle n'|q|n\rangle = \int_{-\infty}^{\infty} dq \psi_{n'}^*(q) q \psi_n(q) \quad \text{for BO} , \quad (4.22)$$

$$\langle n'|q|n\rangle = \int_{-\infty}^{\infty} ds \psi_{n'}^*(s) q(s) \psi_n(s) \quad \text{for ALACM} , \quad (4.23)$$

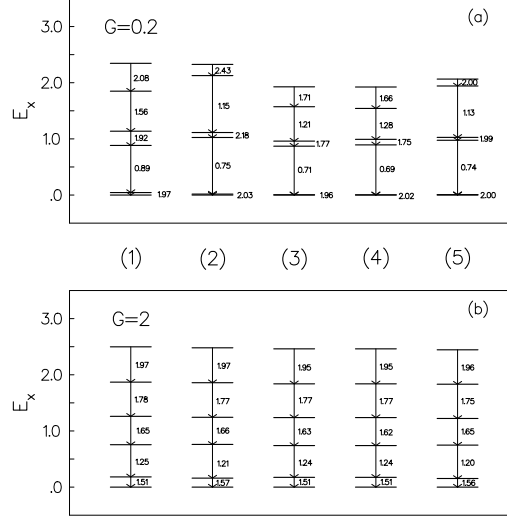


FIG. 7. Spectra up to the fifth excited states for (1) the BO theory without  $\Phi(q)$ , (2) the BO theory with  $\Phi(q)$ , (3) the ALACM theory without  $\Phi(s)$ , (4) the ALACM theory with  $\Phi(s)$ , and (5) the exact calculation. Figure (a) is for  $G = 0.2$  and (b) for  $G = 2$ . The numbers next to the arrows denote The values of the transition matrix element  $|\langle n|q|n+1\rangle|$ .

where the wave functions  $\psi(q)$  and  $\psi(s)$  are normalised with respect to the coordinates  $q$  and  $s$ , respectively. Again, for the case of weak pairing, the amplitude between the first and second excited states is overestimated in BO theory (1) due to too strong mixing of two minima. This is corrected in ALACM (3), (4) and in BO with gauge potential (2).

Table I shows the expectation values of the decoupling measure  $D$  with respect to individual states,

$$\langle n|D|n\rangle = \int_{-\infty}^{\infty} ds \psi_n^*(s)D(s)\psi_n(s) . \quad (4.24)$$

These values are about 7 orders of magnitude smaller for the case of strong pairing  $G = 2$  compared to the weak pairing  $G = 0.2$ . For the weak pairing force, it turns out that all states considerably suffer bad decoupling. Surprisingly, still we have obtained reasonable agreement for the low-lying spectra and transition amplitudes.

## V. CONCLUSION

We have investigated a simple system with level crossings where the monopole pairing interaction plays an important role and the potential landscape exhibits multiple local minima. To apply the ALACM theory, canonical coordinates and a classical Hamilton's equation have been introduced by parametrisation of the time-dependent states. We have done this in two different ways. One is based on the time-dependent mean-field (BCS) theory in which states are not eigenstates of particle number. It is inevitable that this introduces

TABLE I. Expectation values of the decoupling measure  $\langle n|D|n\rangle$  with respect to individual eigenfunctions for cases (3) and (4) in Fig. 7. See the main text and the caption of Fig. 7 for more details.

$n$	$G = 0.2$		$G = 2$	
	(3)	(4)	(3)	(4)
1	57	45	$3.97 \times 10^{-6}$	$3.98 \times 10^{-6}$
2	55	45	$1.72 \times 10^{-6}$	$1.71 \times 10^{-6}$
3	172	162	$3.17 \times 10^{-6}$	$3.17 \times 10^{-6}$
4	181	167	$3.19 \times 10^{-6}$	$3.19 \times 10^{-6}$
5	8.0	7.1	$1.01 \times 10^{-6}$	$1.00 \times 10^{-6}$
6	119	125	$2.99 \times 10^{-6}$	$2.99 \times 10^{-6}$

a Nambu-Goldstone (NG) mode (pairing rotation) in the theory. We have developed the constrained local harmonic formalism which can treat this spurious component and find a path orthogonal to the NG mode in the configuration space. The other is based on the exact time-dependent Schrödinger equation. It is possible to derive a classical Hamilton's equation for a simple two-level system by regarding the mixing angle and the relative phase as canonical variables, though this becomes more complicated when the number of levels increases. In this parametrisation, states are always eigenstates of particle number and there is no NG mode.

Using the mean-field parametrisation (neglecting Fock terms), we have found that the system exhibits completely different collective paths depending on the strength of pairing force. For a weak pairing force, the collective path cannot connect one local minimum with another. On the other hand, a path which connects two local minima is obtained for the case of a strong pairing force. In this model, different local minima correspond to different configurations of valence particles. Therefore, the strength of pairing force determines either adiabatic or diabatic behaviours of the system.

Using the parametrisation of the exact time-dependent Schrödinger equation, if  $G \neq 0$ , a collective path starting from a local minimum always passes through a saddle point and reach the other minimum. For the strong pairing force, the path is very smooth and is well decoupled from the other degree of freedom orthogonal to the path. However, for the weak pairing force, the path shows a peculiar behaviour (back-bending) on the way where the decoupling is very bad. This is qualitatively consistent with the mean-field results.

We have requantised the 1-dimensional collective Hamiltonian and compared the spectra and transition matrix elements with exact calculations. For the strong pairing force, the agreement is excellent for any kind of adiabatic approximation (BO, ALACM). However, for the weak pairing, the BO approximation fails to reproduce the qualitative features of exact spectra, while the ALACM well reproduces the low-lying spectra and transition amplitudes. The agreement becomes worse for the higher-lying states beyond a barrier height between two local minima. The theory is based on the adiabatic assumption in which Hamiltonians are expanded with respect to momentum up to second order. Thus, this disagreement may come from the higher-order terms we have neglected, because the higher-lying states are supposed to have larger momenta.

We have also discussed the effect of gauge potentials arising from change of intrinsic

states along the path. Inclusion of these potentials turns out to improve the BO calculations considerably but to leave the ALACM results almost unchanged.

The authors of Ref. [8] have studied the same model Hamiltonian and concluded that for the case of a weak pairing force the adiabatic approach (BO approximation) is not appropriate for describing the system and the diabatic approach is needed. However, one should bear in mind that, in the BO approximation, the collective coordinate  $q$  was chosen by assuming that the motion of valence particles described by  $(\xi, \pi)$  is much faster than the motion along  $q$ . This is apparently not the case for the weak pairing  $G \ll 1$ . In our adiabatic approach, all degrees of freedom are treated equivalently, taking account of the mass tensor in the multi-dimensional configuration space. Thus the collective path is very much different from the one in the BO approximation for the case of weak pairing. Actually, the collective path turns out to represent the completely diabatic dynamics in some cases. Therefore, if one has a decoupled path determined by the system itself, the *adiabatic* theory may account for the *diabatic* dynamics.

For the practical applications of the ALACM theory, generally speaking, it is not easy to solve the constraints about the NG mode explicitly. Since nuclei show many kinds of symmetry breaking (translational symmetry, rotational symmetry, gauge symmetry), the constrained local harmonic formalism discussed in Sec. II B will be very useful in such cases. We shall apply this method to more realistic problems in the near future.

In conclusion, the ALACM improves on the conventional BO theory. It works well even when the mass of valence Hamiltonian is smaller than that of the core Hamiltonian, because, in principle, the ALACM treats all degrees of freedom equivalently. The ALACM fails to reproduce properties of higher-lying states in the case of weak pairing. This is definitely due to a limitation of the adiabatic theory. Upon requantisation, a reasonable agreement with the exact calculation has been achieved in both cases of strong and weak pairing forces, at least for the low-lying states.

## ACKNOWLEDGMENTS

This work was supported by a research grant from the Engineering and Physical Sciences Research Council (EPSRC) of Great Britain.

## REFERENCES

- [1] A. Klein, N.R. Walet and G. Do Dang, Ann. Phys. **208** (1991) 90.
- [2] N.R. Walet, G. Do Dang and A. Klein, Phys. Rev. **C43** (1991) 2254.
- [3] N.R. Walet, A. Klein and G. Do Dang, Phys. Rev. **C45** (1992) 249.
- [4] D.L. Hill and J.A. Wheeler, Phys. Rev. **89** (1953) 1102.
- [5] R. Bengtsson and W. Nazarewicz, Z. Phys. **A334** (1989) 269.
- [6] G. Bertsch, *Frontiers and borderlines in many-particle physics*, (Enrico Fermi School, CIV Corso, 1988), p.41.
- [7] P.A.M. Dirac, *Lectures on Quantum Mechanics*, (Belfer Graduate School of Science, Yeshiva University, New York, 1964).
- [8] T. Fukui, M. Matsuo, K. Matsuyanagi, Prog. Theor. Phys. **85** (1991) 281.
- [9] J.-P. Blaizot and G. Ripka, *Quantum Theory of Finite Systems*, (The MIT Press, Cambridge, Massachusetts, 1986), p.298.
- [10] D.J. Thouless, Nucl. Phys. **21** (1960) 225.